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Some notes on summation by parts time integration methods

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ABSTRACT

Some properties of numerical time integration methods using summation by parts (SBP) operators and simultaneous approximation terms are studied. These schemes can be interpreted as implicit Runge-Kutta methods with desirable stability properties such as *A*-, *B*-, *L*-, and algebraic stability [1–4]. Here, insights into the necessity of certain assumptions, relations to known Runge-Kutta methods, and stability properties are provided by new proofs and counterexamples. In particular, it is proved that a) a technical assumption is necessary since it is not fulfilled by every SBP scheme, b) not every Runge-Kutta scheme having the stability properties of SBP schemes is given in this way, c) the classical collocation methods on Radau and Lobatto nodes are SBP schemes, and d) nearly no SBP scheme is strong stability preserving.

Known results on SBP SAT schemes

In order to solve an ordinary differential equation (ODE)

$$\forall t \in (0,T) : u'(t) = f(t, u(t)), \qquad u(0) = u_0, \tag{1}$$

a grid $0 \le \tau_1 < \ldots < \tau_s \le T$ is introduced and the numerical solution is approximated pointwise as $u_i = u(\tau_i)$ and $f_i = f(\tau_i, u_i)$. Summation by parts (SBP) operators can be defined as follows, cf [5–7].

Definition 1.1. An SBP operator of order $p \in \mathbb{N}$ on $[0,T]$ consists of

- a discrete operator D approximating the derivative $Du \approx u'$ with order of accuracy p,
- a symmetric and positive definite discrete mass/norm matrix M approximating the L^2 scalar product $u^T M v \approx \int_0^T u(t) v(t) \mathrm{d}t$,
- and interpolation vectors t_L, t_R approximating the interpolation to the boundary as $t_L^T u \approx u(0)$, $t_R^T u \approx u(T)$ with order of accuracy at least p, such that

$$MD + D^T M = t_R t_R^T - t_L t_L^T. \tag{2}$$

SBP operators mimic integration by parts discretely via the summation by parts property (2). An SBP time discretisation using a simultaneous approximation term (SAT) of (1) with parameter $\sigma \in \mathbb{R}$ is [1–3].

$$Du = f + \sigma M^{-1} t_L \left(u_0 - t_L^T u\right). \tag{3}$$

Most stability results have been achieved for the choice $\sigma = 1$, i.e.

$$Du = f + M^{-1} t_L \left(u_0 - t_L^T u\right). \tag{4}$$

Hence, this discretisation will be considered in the following. The numerical solution at $t = T$ is given by $t_R^T u$, where u solves (4). The interval $[0,T]$ can also be partitioned into multiple subintervals/blocks such that multiple steps of this procedure are used sequentially.

In order to guarantee that (4) can be solved for a dissipative linear scalar problem, the following assumption is introduced [1].

Assumption 1.2. For $\sigma > \frac{1}{2}$, all eigenvalues of $D + \sigma M^{-1} t_L t_L^T$ have strictly positive real part.

The following characterisation of (4) as Runge-Kutta method has been developed in Ref. [3].

Theorem 1.3. *If Assumption 1.2 is satisfied, (4) is equivalent to an implicit Runge-Kutta method with the following Butcher coefficients, where* 1 *denotes also the vector* $(1, \ldots, 1)^T \in \mathbb{R}^s$.

$$A = \frac{1}{T}\left(D + M^{-1} t_L t_L^T\right)^{-1} = \frac{1}{T}\left(MD + t_L t_L^T\right)^{-1} M, \quad b = \frac{1}{T} M 1, \quad c = \frac{1}{T}(\tau_1, \ldots, \tau_s)^T. \tag{5}$$

The factor $\frac{1}{T}$ is needed since Runge-Kutta coefficients are normalised to the interval $[0,1]$.

In order to make this article sufficiently self-contained, some classical stability properties of Runge-Kutta methods will be recalled briefly, cf. [8, sections IV.3 and IV.12]. The absolute value of solutions of the scalar linear ODE $u'(t) = \lambda u(t)$, $u(0) = u_0 \in \mathbb{C}$, $\lambda \in \mathbb{C}$, cannot increase if

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$\mathrm{Re}\lambda \le 0$. The numerical solution after one time step of a Runge-Kutta method with Butcher coefficients A, b, c is $u_+ = R(\lambda\, \Delta t) u_0$, where

$$R(z) = 1 + z b^T (\mathrm{I} - zA)^{-1} 1 = \frac{\det(\mathrm{I} - zA + z 1 b^T)}{\det(\mathrm{I} - zA)} \tag{6}$$

is the *stability function* of the Runge-Kutta method. The stability property is mimicked discretely as $u_+ \le u_0$ if $R(\lambda\, \Delta t) \le 1$.

Definition 1.4. A Runge-Kutta method with stability function $R(z)$ is A-stable, if $R(z) \le 1$ for all $z \in \mathbb{C}$ with $\mathrm{Re}(z) \le 0$. The method is L-stable, if it is A-stable and $\lim_{z\to\infty} R(z) = 0$.

Hence, A-stable methods are stable for every time step $\Delta t > 0$ and L-stable methods damp out stiff components corresponding to $\lambda = -x$ with large $x \in \mathbb{R}$ sufficiently fast.

Another classical stability property is connected with possibly nonlinear problems (1) in Hilbert spaces satisfying a *one-sided Lipschitz condition*

$$\forall t, u, v: \quad \langle f(t,u) - f(t,v),\; u - v \rangle \le \nu \|u - v\|^2, \tag{7}$$

where $\nu \in \mathbb{R}$ is the *one-sided Lipschitz constant* of f. This condition gives some bounds on the growth rate of the difference between two solutions. In particular, the distance between two solutions cannot increase if $\nu \le 0$.

Definition 1.5. A Runge-Kutta method is B-stable, if the contractivity condition (7) with $\nu \le 0$ implies $\|u_+ - v_+\| \le \|u_0 - v_0\|$ for all $\Delta t > 0$.

The following stability properties have been obtained in Refs. [2,3].

Theorem 1.6. Suppose that Assumption 1.2 *holds. Then, the SBP SAT scheme* (4) *is A- and L-stable. If the mass matrix M is diagonal, the scheme is also B-stable.*

Assumptions and algebraic stability

In this section, the new results of this short note concerning the necessity of Assumption 1.2 and the necessity of an SBP SAT form for stability properties guaranteed by Theorem 1.6 are presented.

Assumption on Eigenvalues of $D + \sigma M^{-1} t_L t_L^T$

Assumption 1.2 has been proved for classical second order SBP operators in Ref. [1] and for SBP operators on Gauss, Radau, and Lobatto quadrature nodes in Ref. [4]. It has been examined numerically for other classical finite difference SBP operators in Ref. [1]. Since Assumption 1.2 holds for all known SBP SAT schemes investigated in Refs. [1–4], it is interesting to know whether it follows from properties of SBP operators.

Theorem 2.1. *There are SBP operators that do not satisfy* Assumption 1.2

Proof. *Consider the operators*

$$D = \begin{pmatrix} -2 & 1 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & -1 & 2 \end{pmatrix}, \quad M = \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad t_L = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad t_R = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \tag{8}$$

on the uniform grid with four nodes $0, \frac{1}{3}, \frac{2}{3}, 1$ in $[0,1]$. The SBP property (2) is satisfied, t_L and t_R are exact, and D is a first order accurate SBP derivative operator.

However, $(D + \sigma M^{-1} t_L t_L^T) u = 0$ for $u = (0, -1, 1, 0)^T$. Thus, zero is an eigenvalue of $D + \sigma M^{-1} t_L t_L^T$ for all $\sigma \in \mathbb{R}$. □

Algebraic stability

Many stability properties such as A- and B-stability are satisfied if the following algebraic criterion is fulfilled by the coefficients of a Runge-Kutta method [8, Theorem 12.4].

Definition 2.2. A Runge-Kutta method with Butcher coefficients A, b, c is algebraically stable, if $\forall i: b_i \ge 0$ and the matrix $\operatorname{diag}(b) A + A^T \operatorname{diag}(b) - b b^T$ is positive semidefinite.

It has been noted in Ref. [3] that an SBP SAT scheme (4) with diagonal M is algebraically stable, since the nodes τ_i are pairwise distinct, i.e. the corresponding Runge-Kutta method is nonconfluent. In that case, B- and algebraic stability are equivalent [8, Corollary 12.14]. This can also be proved directly, cf. [3, Theorem 5.8].

It is interesting to know whether all Runge-Kutta methods with stability properties guaranteed by Theorem 1 can be constructed as SBP SAT schemes. Since those schemes are L-stable, the classical Gauss collocation schemes (which are not L-stable) cannot be constructed in this way, cf. [3]. However, there is

Theorem 2.3. *Consider a Runge-Kutta method and the statements*

i) *The Runge-Kutta method is A-, L-, B-, and algebraically stable with pairwise distinct nodes $c_i \in [0,1]$, only positive quadrature weights b_i, and invertible matrix A.*
ii) *The Runge-Kutta method is given via* Theorem 1.3 *by SBP SAT schemes* (4) *with at least first order accurate operators satisfying* Assumption 1.2.

Theorem 1.6 *and the preceeding discussion show that ii) and "M is diagonal" imply i). However, i) does not imply ii).*

Proof. *The following example has been constructed using the W-transformation* [8, Sections IV.5, IV.13, and IV.14]. *Consider the Runge-Kutta method with coefficients*

$$A = \frac{1}{48}\begin{pmatrix} 27 & -33 - 6\sqrt{6} & -3 & 9 + 6\sqrt{6} \\ -7 + 2\sqrt{6} & 33 & -9 - 2\sqrt{6} & -1 \\ 7 & 3 + 2\sqrt{6} & 33 & -11 - 2\sqrt{6} \\ 21 - 6\sqrt{6} & 21 & -21 + 6\sqrt{6} & 27 \end{pmatrix}, \quad b = \frac{1}{8}\begin{pmatrix} 1 \\ 3 \\ 3 \\ 1 \end{pmatrix}, \quad c = \frac{1}{3}\begin{pmatrix} 0 \\ 1 \\ 2 \\ 3 \end{pmatrix}. \tag{9}$$

Then, the algebraic stability matrix $\operatorname{diag}(b) A + A^T \operatorname{diag}(b) - b b^T$ has the eigenvalues $\frac{5}{8}, \frac{3}{8}$, and zero (twofold). Hence, the Runge-Kutta method is algebraically stable (because $b_i > 0$ is satisfied additionally) and therefore also A- and B-stable. Its stability functions

$$R(z) = \frac{\det(\mathrm{I} - zA + z 1 b^T)}{\det(\mathrm{I} - zA)} = \frac{12 - 18z + 3z^2 + 3z^3}{12 - 30z + 27z^2 - 11z^3 + 2z^4}, \tag{10}$$

fulfils $\lim_{z\to\infty} R(z) = 0$. Thus, the scheme is also L-stable.

It suffices to consider $T = 1$. If the scheme is given by an SBP SAT method (4) via Theorem 1.3, $b = M1$ and $A = (D + M^{-1} t_L t_L^T)^{-1}$. The SBP property (2) yields $A^{-1} = -M^{-1} D^T M + M^{-1} t_R t_R^T$. Because of consistency, $D1 = 0$ and $t_R^T 1 = 1$. Hence, $1^T M A^{-1} = t_R^T$. Inserting $M1 = b$ results in

$$t_R = A^{-T} b = \frac{1}{16}\Big(-4 + \sqrt{6}, -\sqrt{6}, 12 - \sqrt{6}, 8 + \sqrt{6} \Big)^T. \tag{11}$$

Similarly, consistency of D and t_L implies

$$A^{-1} 1 = \big(D + M^{-1} t_L t_L^T\big) 1 = M^{-1} t_L \Leftrightarrow t_L = M A^{-1} 1. \tag{12}$$

t_R defined by (11) is first order accurate, i.e. $t_R^T 1 = 1$ and $t_R^T c = 1$. The same accuracy of t_L requires

$$t_L^T 1 = 1, \quad t_L^T c = 0. \tag{13}$$

Because of (12), D can be written as

$$D = A^{-1} - M^{-1} t_L t_L^T = A^{-1} - A^{-1} 1 t_L^T. \tag{14}$$

Since $M \in \mathbb{R}^{4\times 4}$ should be symmetric, it is determined by ten real parameters, e.g. M_{11}, M_{12}, M_{13}, M_{14}, M_{22}, M_{23}, M_{24}, M_{33}, M_{34}, M_{44}. t_R is given explicitly by (11), t_L depends linearly on M via (12), and D is given via an affine-linear function of M in (14).

The accuracy conditions (13) are linear in t_L and hence linear in M. They can be used to eliminate two parameters, e.g. M_{11} and M_{12}. Then, the SBP property (2) is a system of 16 equations that are quadratic in the parameters M_{ij}. This system can be solved uniquely, which has been verified using the function Reduce of Mathematica [9]. For this unique solution, one eigenvalue of M is zero. Thus, M is not positive definite, in contradiction to the assumptions.

Classical collocation methods

In Ref. [3], it has been shown that the SBP SAT scheme with Lobatto quadrature on four nodes corresponds to the classical Lobatto IIIC method with $s = 4$. It has been mentioned that this is similar for the Radau IA and Radau IIA schemes. However, to the authors knowledge, no general Proof of this result has been given up to now. To prove it, the classical conditions

$$C(\eta) : \sum_{j=1}^{s} a_{i,j} c_j^{q-1} = \frac{1}{q} c_i^q, i \in \{1,\dots,s\},\ q \in \{1,\dots,\eta\}, \tag{15}$$

$$D(\zeta) : \sum_{i=1}^{s} b_i c_i^{q-1} a_{i,j} = \frac{1}{q} b_j \left(1 - c_j^q\right), j \in \{1,\dots,s\},\ q \in \{1,\dots,\zeta\}, \tag{16}$$

will be used.

Theorem 3.1. *The SBP SAT scheme* (4) *using left Radau, right Radau, or Lobatto quadrature correspond to the classical Radau IA, Radau IIA, or Lobatto IIIC Runge-Kutta methods for all orders of accuracy.*

Proof. *It suffices to consider the case $T = 1$, i.e. the time interval $[0,1]$.*

The weights and nodes of the left Radau quadrature (left endpoint 0 included) are the weights b_i and nodes c_i of the Radau IA method. The matrix A of the Radau IA method is determined uniquely by the condition $D(s)$, i.e. $D(\zeta)$ with $\zeta = s$ in (16) [8, section IV.5]. Hence, it suffices to prove that the SBP SAT method satisfies $D(s)$, which can be written using $M = \operatorname{diag}(b)$ as

$$A^T M c^{q-1} = \frac{1}{q} M (1 - c^q) \Leftrightarrow q M c^{q-1} = A^{-T} M (1 - c^q), \tag{17}$$

where the exponentiation c^q is performed pointwise. Inserting A from (5) yields

$$q M c^{q-1} = \left(D^T M + t_L t_L^T\right)(1 - c^q). \tag{18}$$

This is equivalent to

$$\forall v: \quad q v^T M c^{q-1} = v^T \left(D^T M + t_L t_L^T\right)(1 - c^q), \tag{19}$$

where v is any polynomial of degree $\le s-1$, evaluated at the nodes c_i. Since the left endpoint 0 is included,

$$v^T t_L t_L^T (1 - c^q) = v(0)\,(1 - 0^q) = v(0). \tag{20}$$

The Radau quadrature is exact for polynomials of degree $\le 2s-2$. Hence, for every $q \in \{1,\dots,s\}$,

$$q v^T M c^{q-1} = q \int_0^1 v(t) t^{q-1} \mathrm{d}t \tag{21}$$

and (using integration by parts)

$$v^T D^T M (1 - c^q) = \int_0^1 v'(t)(1 - t^q)\mathrm{d}t = -v(0) + q \int_0^1 v(t) t^{q-1} \mathrm{d}t, \tag{22}$$

proving $D(s)$.

The weights and nodes of the right Radau quadrature (right endpoint 1 included) are the weights b_i and nodes c_i of the Radau IIA method. The matrix A of the Radau IIA method is determined uniquely by the condition $C(s)$, i.e. $C(\eta)$ with $\eta = s$ in (15) [8, section IV.5]. Hence, it suffices to prove that the SBP SAT method satisfies $C(s)$, which can be written using $M = \operatorname{diag}(b)$ as

$$A c^{q-1} = \frac{1}{q} c^q \Leftrightarrow q M c^{q-1} = M A^{-1} c^q, \tag{23}$$

where the exponentiation c^q is again performed pointwise. Inserting A from (5), this is equivalent to

$$\forall v: \quad q v^T M c^{q-1} = v^T \left(M D + t_L t_L^T\right) c^q, \tag{24}$$

where v is any polynomial of degree $\le s-1$, evaluated at the nodes c_i. Using the SBP property (2), this can be rewritten as

$$\forall v: \quad q v^T M c^{q-1} = v^T \left(-D^T M + t_R t_R^T\right) c^q. \tag{25}$$

Since the right endpoint 1 is included,

$$v^T t_R t_R^T c^q = v(1)\,1^q = v(1). \tag{26}$$

Using the exactness of the Radau quadrature for polynomials of degree $\le 2s-2$, for every $q \in \{1,\dots,s\}$,

$$q v^T M c^{q-1} = q \int_0^1 v(t) t^{q-1} \mathrm{d}t \tag{27}$$

and (using integration by parts)

$$-v^T D^T M c^q = -\int_0^1 v'(t) t^q \mathrm{d}t = -v(1) + q \int_0^1 v(t) t^{q-1} \mathrm{d}t, \tag{28}$$

proving $C(s)$.

Finally, the weights and nodes of the Lobatto quadrature (left and right endpoints $0, 1$ included) are the weights b_i and nodes c_i of the Lobatto IIIC method. The matrix A of the Lobatto IIIC method is determined uniquely by the condition $C(s-1)$ and $a_{i,1} = b_1, i \in \{1,\dots,s\}$ [8, section IV.5]. Since the order of accuracy of the SBP operator is $s-1$, $C(s-1)$ is satisfied [3, Lemma 5.3]. This can also be proved using similar manipulations as above. Hence, it remains to show $a_{i,1} = b_1, i \in \{1,\dots,s\}$. Since D is exact for constants, $t_L = (1, 0, \dots, 0)^T$, and $M = \operatorname{diag}(b_1,\dots,b_s)$,

$$\left(D + M^{-1} t_L t_L^T\right) 1 = 0 + M^{-1} t_L = b_1^{-1} t_L. \tag{29}$$

Therefore, $(a_{i,1})_{i=1}^s = A t_L = \left(D + M^{-1} t_L t_L^T\right)^{-1} t_L = b_1 1$, proving $a_{i,1} = b_1, i \in \{1,\dots,s\}$. □

Strong stability preservation

Another desirable stability property of time integration methods is that they are strong stability preserving (SSP), i.e. that they preserve convex stability properties of the explicit Euler method [10].

Definition 4.1. A numerical time integration method is called strongly stable for a given convex functional η if $\eta(u_+) \le \eta(u_0)$, possibly using some time step restriction of the form $0 < \Delta t \le \Delta t_{\max}$.

A numerical time integration method is called strong stability preserving with SSP coefficient $c > 0$, if $\eta(u_+) \le \eta(u_0)$ for all time steps $0 < \Delta t \le c\,\Delta t_E$ whenever the explicit Euler method is strongly stable for the convex functional η and time steps $0 < \Delta t \le \Delta t_E$.

Typical convex functionals η considered for SSP methods are the norm in a Hilbert space for dissipative operators or the total variation seminorm for semidiscretisations of scalar conservation laws.

Theorem 4.2. *No SBP SAT scheme (4) whose SBP operator has a diagonal norm matrix, satisfies Assumption 1.2, and*

a) *is either at least second order accurate*
b) *or is at least first order accurate and contains at least one of the end points* $0, 1$ *in the nodes* c_i *can be strong stability preserving.*

Proof. *An SSP scheme must satisfy* $\forall i, j \in 1, \ldots, s : a_{i,j} \geq 0$ [10, *Observation* 5.2].

If the SBP operator is at least second order accurate, the corresponding Runge-Kutta method satisfies $C(2)$ [3, Lemma 5.3], i.e. $\sum_{j=1}^{s} a_{i,j} = c_i$ and $\sum_{j=1}^{s} a_{i,j} c_j = \frac{1}{2} c_i^2$ for $i \in \{1, \ldots, s\}$. Subtracting the second equation from the first one multiplied by c_i yields

$$\sum_{j=1}^{s} a_{i,j} (c_i - c_j) = \frac{1}{2} c_i^2, \quad i \in \{1, \ldots, s.\} \tag{30}$$

If $a_{i,j}$ were non-negative, the left hand side would be non-positive for $i = 1$ (since $c_j \geq c_1$) and thus zero. Hence, the first row of A would be zero, which is impossible, because A is invertible.

If the SBP operator is at least first order accurate, the corresponding Runge-Kutta method satisfies $C(1)$ and $D(1)$ [3, Lemma 5.3 and Lemma 5.4], i.e.

$$\sum_{j=1}^{s} a_{i,j} = c_i, \; i \in 1, \ldots, s, \qquad \sum_{i=1}^{s} b_i a_{i,j} = b_j (1 - c_j), \; j \in 1, \ldots, s. \tag{31}$$

If the left endpoint $0 = c_1$ is contained in the nodes, non-negativity of all $a_{i,j}$ and $C(1)$ imply $\forall j \in \{1, \ldots, s\} : a_{1,j} = 0$. Similarly, if the right endpoint $c_s = 1$ is contained in the nodes, non-negativity of all $a_{i,j}$ and $D(1)$ imply $\forall i \in \{1, \ldots, s\} : a_{i,s} = 0$. But A cannot have a zero row or column because it is invertible. □

Remark 4.3. Classical finite difference SBP operators and those based on Radau or Lobatto quadrature include at least one endpoint and can thus not result in SSP schemes. The SBP SAT scheme (4) on two Gauss nodes does not contain an endpoint and has a first order accurate derivative operator. Nevertheless, the scheme is not SSP, since the corresponding matrix A has a negative entry.

Example 4.4. There is a first order accurate SBP operator with diagonal norm matrix not including any boundary node such that the resulting Runge-Kutta method given by Theorem 1.3 is SSP. Indeed, choose $T = 1$ and

$$D = \frac{1}{128} \begin{pmatrix} -2079 & 3646 & -1567 \\ 271 & -1054 & 783 \\ -479 & 446 & 33 \end{pmatrix}, \quad M = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad t_L = \begin{pmatrix} 3 \\ -3 \\ 1 \end{pmatrix}, \quad t_R = \frac{1}{16} \begin{pmatrix} -15 \\ 14 \\ 17 \end{pmatrix},$$
$$c = \frac{1}{4} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}, \quad A = \left(D + M^{-1} t_L t_L^T \right)^{-1} = \frac{1}{20000} \begin{pmatrix} 2725 & 2180 & 95 \\ 4390 & 5512 & 98 \\ 3495 & 6796 & 4709 \end{pmatrix}. \tag{32}$$

The operators D, t_L, t_R are exact for polynomials of degree one, Assumption 1.2 has been verified numerically for $\sigma \in (1/2, 2)$, A and b have only non-negative entries, and the scheme is strong stability preserving with SSP coefficient ≈ 1.35, computed using NodePy [11].

Conflict of interest

I declare that there is no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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